

Coupling Between Precipitation and Plastic Deformation During Electromigration in a Passivated Al (0.5wt%Cu) Interconnect

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ABSTRACT

In the present paper the evolution of the dislocation structure during electromigration in different regions along the Al(Cu) interconnect line is considered. It is shown that plastic deformation increases in the regions close to cathode end of the interconnect line. A coupling between the dissolution, growth and re-precipitation of Al₂Cu precipitates and the electromigration-induced plastic deformation of grains in interconnects is observed. Possible mechanism of the Cu doping effect on the improved electromigration resistance of the Al(Cu) interconnects is discussed.

INTRODUCTION

The scaling of device dimensions with a simultaneous increase in functional density imposes a challenge to materials technology and reliability of interconnects^{1,2}. Although the general mechanism of electromigration is understood³⁻⁵, the effect of the atomic flow on the local metallic line microstructure is largely unknown. Recently white beam X-ray microdiffraction⁶⁻¹⁷ was used to probe microstructure in interconnects. The first quantitative analysis of the dislocation structure in individual grains of a polycrystalline interconnect line was performed in¹⁵⁻¹⁷ and it was shown that dislocations with their lines almost parallel to the current flow direction are formed first. Electromigration in Al(Cu) interconnects and the effects of Cu were studied extensively since 70's^{3,4}. Recent measurements of precipitate evolution during electromigration in Al (Cu) interconnects¹⁷⁻²¹, in agreement with earlier results of Rosenberg³ and Hu *et al*⁴ indicates that Cu is preferentially depleted from the cathode end of the line and accumulates at the anode. However it is still not completely understood why doping with small amount of Cu greatly improves the electromigration resistance of Al-based interconnect lines. In the present paper we consider a model describing the possible correlation between Cu drift, precipitation and formation of dislocations in an Al(Cu) interconnect line.

EXPERIMENTAL

Data collection has been carried out at the X-ray microdiffraction end-station on beamline 7.3.3 at the Advanced Light Source. The sample is a patterned Al (0.5% wt.

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Cu) line (length: 30 μm , width: 4.1 μm , thickness: 0.75 μm) sputter deposited on a Si wafer and buried under a glass passivation layer (0.7 μm thick). Electrical connections to the line are made through unpassivated Al (Cu) pads connected to the sample by W vias. Details on the experimental setting and data collection can be found elsewhere⁴⁻⁶. A qualitative description and semi-quantitative interpretation of the entire data set collected for the present sample can be found in recent articles^{14, 15}. The dislocation structure was determined by the analysis of the intensity distribution of the reflections observed in the experimental Laue images^{16, 17, 23}.

RESULTS AND DISCUSSION

In agreement with the previous study¹³⁻¹⁷ white beam analysis of plastic deformation in the Al(Cu) interconnect line demonstrates that the amount of plastic slip increases when the probing location approaches the cathode. The slip systems with dislocation lines almost parallel to the direction of current flow are activated first¹⁵⁻¹⁷. Near the ends of the line plastic activity is coupled with the depletion of Cu from the cathode end of the line. There is practically no plastic activity in the “near anode” end of the line¹⁷.

Such peculiarities in the plastic deformation behavior at the “near anode/cathode” regions can be understood taking into account that Cu is preferentially depleted from the cathode region of the interconnect^{3, 4, 18-20}. Al-Cu alloys are known to demonstrate strong tendency to short range order with strong preference to unlike neighbors. After quenching from the solid solution range across the solvus, decomposition occurs via a sequence of metastable phases prior to the formation of the equilibrium precipitate Al_2Cu ²¹⁻²⁵. Cu rich clusters are known to form during aging at or near room temperature throughout the alloy. These clusters are usually referred to as “GP zones”. These are the mixture of single and multiple {100} Cu rich planes. There is no apparent barrier to GP zone nucleation²⁵. It is commonly accepted that in such alloys the sequence of phase transformations is: $\text{GP1} \Rightarrow \text{GP2 (or } \theta'') \Rightarrow \theta' \Rightarrow \theta$. GP1 are assumed to consist of a single layer of pure Cu on (100) plane. Due to smaller size of the Cu atoms, the surrounding Al planes collapse towards the Cu layer. GP2 consist of multilayered Cu-rich zones²⁶⁻²⁸. The strains around the zones oscillate with distance from them, and vanish near the fourth or fifth {100} Al plane²². The tetragonal θ phase is the equilibrium precipitate Al_2Cu . The size of clusters changes from several atomic layers to 1-5 nm. Such small size coherent precipitates in Al rich Al-Cu alloys were observed for example, by x-ray or neutron diffuse scattering measurements, high resolution electron microscopy or field ion microscopy²¹⁻²⁸.

The diffusion mechanism in the presence of such precipitates may differ from the diffusion in the homogeneous solid solution. This agrees with the viewpoint¹⁸ which strongly suggests that some transport mechanism other than lattice diffusion controls steady state transport in the interconnect lines. Interestingly, during the time of the electromigration test, there is no visible dislocation activity close to the anode end of the line, while the “near cathode” grain is quickly plastically deformed. The dissolution kinetics of Al_2Cu precipitates near the cathode end and its migration in the interconnect line is coupled with the plastic deformation activity. To interpret such a behavior we

propose a generalization of the model of electromigration-induced Cu motion and precipitation in Al(Cu) interconnects, described in^{3, 4, 18 - 20}, and a mechanism which takes into account the coupling between plastic deformation and precipitation formation, dissolution and migration in different regions of the line.

Dissolution of large size precipitates at the cathode end was described in the number of papers^{3, 4, 18 - 20, 29}. With the decrease of precipitate size they finally reach some critical “nanometer” size (cluster) and start to migrate in the matrix relative to the lattice due to directional diffusion of atoms under applied electric field. Such migration results in the gradual departure (dissolution) of atomic layers of the Al matrix on one side of the precipitate and their simultaneous growth on the opposite side of the precipitate. As a result the precipitate migrates relatively to the matrix in the applied electric field. As is shown below, the velocity of migration, v , is inversely proportional to the precipitate size, $v \propto 1/R$ (see Eq.10). This means that the migration rate is negligible for large precipitates and they just dissolve (in agreement with a number of experimental observations^{4, 18 - 20}). However when the precipitate diameter reduces to the size of about 5-10 atoms the migration rate becomes essential. For such small precipitate size the diffusivity related to precipitate migration is about 10^{-3} times smaller than the diffusivity of individual Cu atoms (such ratio between the bulk diffusivity and experimentally observed during electromigration was found in¹⁸).

Diffusivity for Cu and Al atoms at the matrix/precipitate interface is different. This is why an applied electric field causes more rapid motion of one type of atoms along the surface while a different atomic species would move more slowly. This creates an inhomogeneous distribution of interface concentration within the matrix at the precipitate boundary, which in turn causes additional diffusion fluxes. They compensate the difference in diffusivity of Cu and Al atoms. After a relaxation time ε , the process stabilizes and steady state is reached. The relaxation time can be estimated by:

$$\varepsilon \sim R^2 / D_s \quad (1)$$

Here R is the average precipitate size and D_s the interface diffusivity. After that time, the interface concentration distribution becomes stationary and the precipitate/matrix interface migrates with constant velocity in the matrix. We note that for large precipitates this time is huge and such precipitates dissolve rather than migrate (as observed experimentally^{3, 4, 18 - 20}). To quantitatively describe this process, we define the unit vector perpendicular to the precipitate/matrix interface, \mathbf{n}_s . The product $\mathbf{I}_s \mathbf{n}_s$ between \mathbf{n}_s and the surface atomic flux \mathbf{I}_s (across the precipitate surface) gives the number of atoms passing in the near surface region through the unit length tangential to the vector \mathbf{n}_s per unit of time. This flux depends on the coordinate of the position at the surface of the precipitate. This way the number of atoms coming in through some surface element and leaving the precipitate is different. Under the applied electric field such diffusive fluxes result in the motion of atoms from the front to the back side of the precipitate. As a result small coherent precipitates are migrating in the interconnect line (Fig. 1).

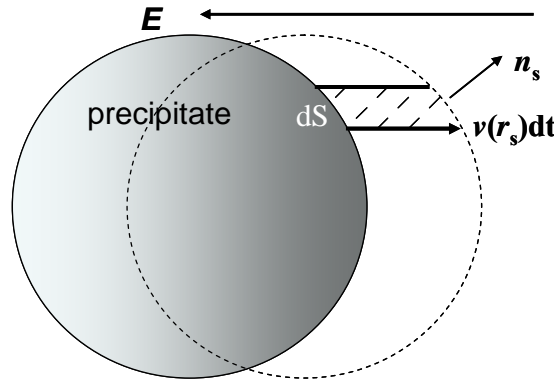


Figure 1. Volume change due to the migration of the surface element of precipitate dS on the distance $\mathbf{v}(\mathbf{r}_s)dt$. \mathbf{n}_s is a surface normal unit vector at the position \mathbf{r}_s at the surface of the precipitate.

This mechanism is especially important at relatively low temperatures when the ratio of surface to volume diffusivity is high, and for small size of precipitates when the ratio of their surface atoms to their volume atoms is not too small. For example for a typical size of Al_2Cu precipitates in the interconnect line of the order of 5 - 10 atoms in diameter the number of surface atoms is approximately equal to their number in the volume of precipitate.

The volume diffusion of Cu and Al atoms under the applied electric field in the interconnect can be written as³⁰

$$\mathbf{I}_i = N_0 c_i \frac{D_i^*}{f_i kT} e Z_i \mathbf{E} \quad (2)$$

Here D_i^* is the volume self-diffusion coefficient for atom i ($i=1, 2$, for Cu and Al respectively), Z_i is an effective charge of ions caused both by the direct force applied to the ion in the electric field \mathbf{E} and by the force of the electron wind, N_0 is a number of atoms per unit volume, c_i concentration of Cu/Al atoms in the alloy, f_i is a correlation factor for ions in the solid solution; e is the electron charge.

The interface diffusion flux \vec{I}_{Si} for Cu and Al atoms of the Al (0.5 wt% Cu) alloy in the electric field \mathbf{E}_s can be written

$$\vec{I}_{Si} = N_0 c_{Si} \frac{D_{Si}^* a}{f_{Si} kT} e Z_{Si} \vec{E}_s \quad (3)$$

Here D_{Si}^* is interface self-diffusion coefficient for atom i , Z_{Si} is effective charge, f_{Si} is a correlation factor; a is the thickness of one atomic surface layer, e is the electron charge. In both equations for volume and surface diffusion all parameters are semi-phenomenological as they are obtained by averaging over possible configurations and depend strongly on the temperature T and the concentration c_i and c_{Si} .

In the coordinate system connected to the interconnect crystal lattice the number of lattice sites is constant. This means that the total flux of Cu and Al atoms and vacancies is equal zero:

$$(\mathbf{I}_{Cu} + \mathbf{I}_{Al} + \mathbf{I}_v) = 0 \quad (4)$$

At the same time the material of the interconnect line (Cu and Al atoms) is moving in the direction opposite to the direction of vacancies flux. Average velocity of atomic movement $\mathbf{v}_a(\mathbf{r})$ is equal to the product of the resulting atomic flux $(\mathbf{I}_{Cu} + \mathbf{I}_{Al})$ and the atomic volume:

$$\mathbf{v}_a(\mathbf{r}) = \omega(\mathbf{I}_{Cu} + \mathbf{I}_{Al}) = -\omega\mathbf{I}_v \quad (5)$$

As the grain boundary is moving together with the materials of the grain the last equation determines the rate of the boundary's displacement in the crystal lattice coordinate system. Vacancy flux corresponds to the particular point of the boundary. The continuous appearance and formation of vacancies in the volume of the crystal grain or at its boundary during diffusion, results in the formation of new and disappearance of existing crystal planes. This means that continuous diffusion deformation of the lattice is taking place.

It is convenient to relate the coordinate system to the boundary of the interconnect line. Continuous reconstruction of the lattice during electromigration results in the motion of each point of the lattice with a velocity $\boldsymbol{\omega}(\mathbf{r})$. If diffusion fluxes are not homogeneous in space, the lattice will not only be moving but deforming as well. Relative volume change of a given volume $\delta V(\mathbf{r})$ during such a deformation is equal to

$$\frac{1}{\delta V} \frac{d\delta V}{dt} = \text{div}\boldsymbol{\omega}(\mathbf{r}) \quad (6)$$

We consider relatively early stages of electromigration when there are no voids or hillocks in the line and number of lattice sites does not change. Under such conditions volume change can take place only if during diffusion some excess number of vacancies gets into the volume δV and simultaneously the same number of atoms leaves this volume. As a result its volume reduces. In the opposite situation when some part of vacancies is leaving the element δV and in exchange new atoms come into this element of the lattice. Such volume will increase. Then the relative volume change of the certain volume $\delta V(\mathbf{r})$ during this process is equal to

$$\frac{1}{\delta V} \frac{d\delta V}{dt} = \omega \frac{\partial N_v}{\partial t} = \omega \text{div}\mathbf{I}_v \quad (7)$$

From the comparison between the last two equations, we obtain the differential equation for the velocity of the lattice displacement, $\boldsymbol{\omega}(\mathbf{r})$:

$$\text{div}\boldsymbol{\omega}(\mathbf{r}) = \omega \text{div}\mathbf{I}_v \quad (8)$$

The problem can be considered as one dimensional so that,

$$\omega_x(x) = \omega[I_{vx}(x) - I_{vx}(x_0)] \quad (9)$$

Here $I_{vx}(x)$ and $I_{vx}(x_0)$ are vacancy fluxes in the position x and at the fixed boundary x_0 . In the stationary stage of precipitate migration, the velocities of different points at the surface of the precipitate are equals, $\mathbf{v}(\mathbf{r}_s) = \mathbf{v}$. Using Darken relations for surface diffusion coefficients³¹ we derive an approximate equation for the velocity of precipitate as follows:

$$\mathbf{v} = -2(1 + \chi) \frac{a}{R} \frac{c_{SCu} Z_{SCu} + c_{SAI} Z_{SAI}}{f_s kT} D_{Seff} e\mathbf{E} \quad (10)$$

Here the effective surface diffusivity is:

$$D_{Seff} = \frac{D_{SCu}^* D_{SAI}^*}{c_{Al} D_{SCu}^* + c_{Cu} D_{SAI}^*} \quad (11)$$

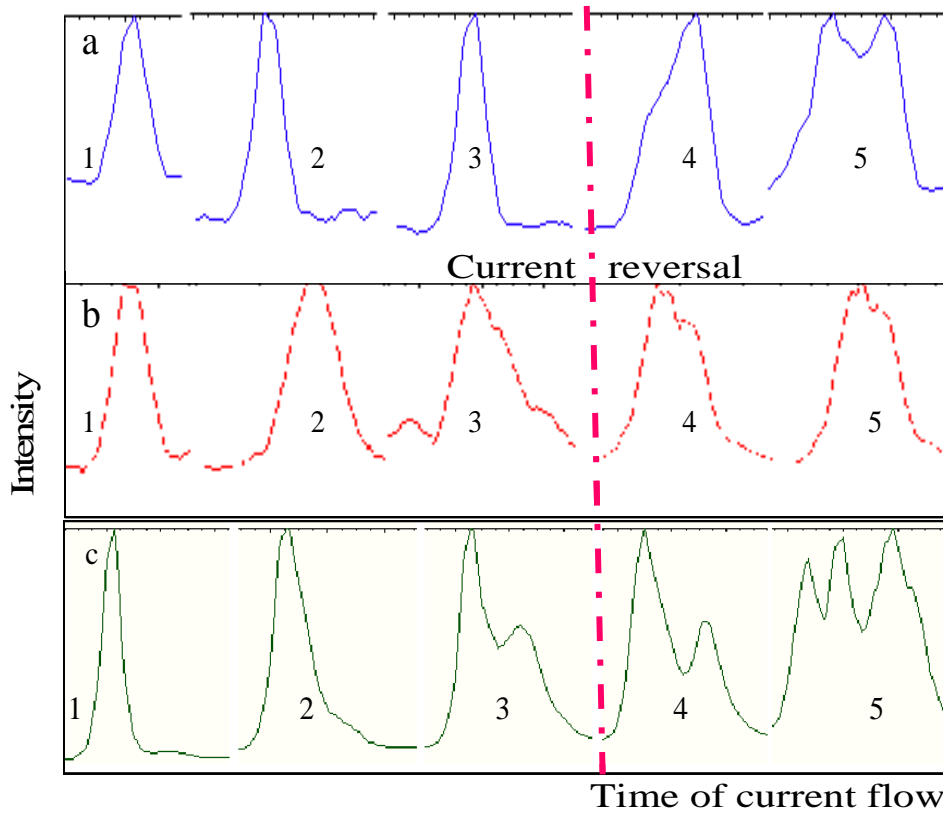


Figure 2. Intensity distribution I (in arbitrary units) along the streak direction (in pixel) for grains located near the anode (a) and cathode (b) ends of the interconnect line before the current reversal and grain (c) in the middle of the interconnect line with time of current flow: 1) initial state before the current flow; 2) 5 hours; 3) 16 hours; 4) 9 hours reversed current; 5) 19 hours reversed current.

From the last two equations, we see that a small addition of Cu atoms with smaller diffusivity relative to the Al matrix atoms may essentially decrease the velocity of electromigration. Such strong decrease of D_{seff} and of v takes place if D_{SCu} is smaller than D_{SAI} so that even the value $c_{Cu}(D_{SAI}/D_{SCu} - 1)$ becomes of the order of unity (or more) at small concentration (0.5wt%). In this region of concentrations when

$1 \gg c_{Cu} \gg \frac{D_{SCu}}{D_{SAI}}$ the velocity of precipitate movement is inversely proportional $\sim c_{Cu}$.

This explains why the addition of small (0.5wt%) amount of Cu strongly improves the reliability of interconnects.

The presence of small precipitates is known to strengthen the Al-based alloys and increase their yield stress. Cu depletion in the near cathode region causes diffusion and partial dissolution of precipitates. Decrease of precipitates size first causes symmetric broadening of the Laue spot, as observed here (Fig.2b, curve2). After precipitates disappear in the near cathode region the critical shear stress decreases and plastic deformation is activated. This is accompanied by streaking and further splitting of Laue spots (Fig2b, curve 3). With the reversal of current flow, Cu concentration in this grain starts to increase and precipitates form again. Critical shear stress is high and plastic activity is suppressed. Reversal of current flow is accompanied with dissolution of precipitates. Critical shear stress decreases and plastic deformation occurs (Fig. 2a, curves 4, 5). This supports the idea¹⁸ that Al (0.5% wt. Cu) interconnects are most reliable when Cu depletion from the cathode end is the slowest.

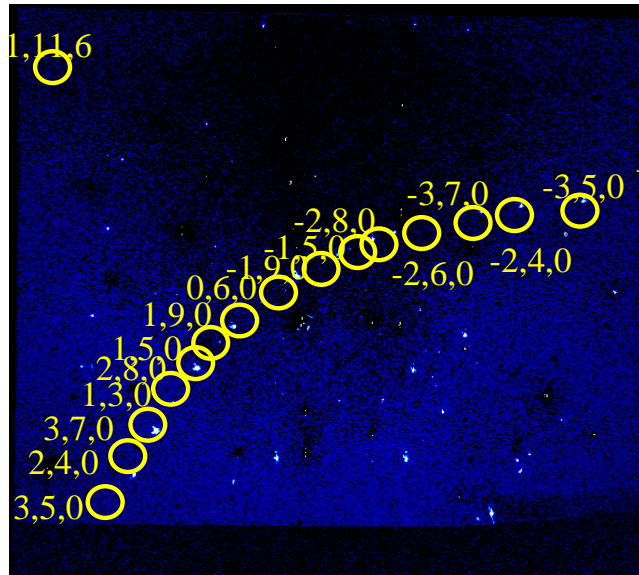


Figure 3. Laue pattern with reflections of Al Cu particle in the metallization.

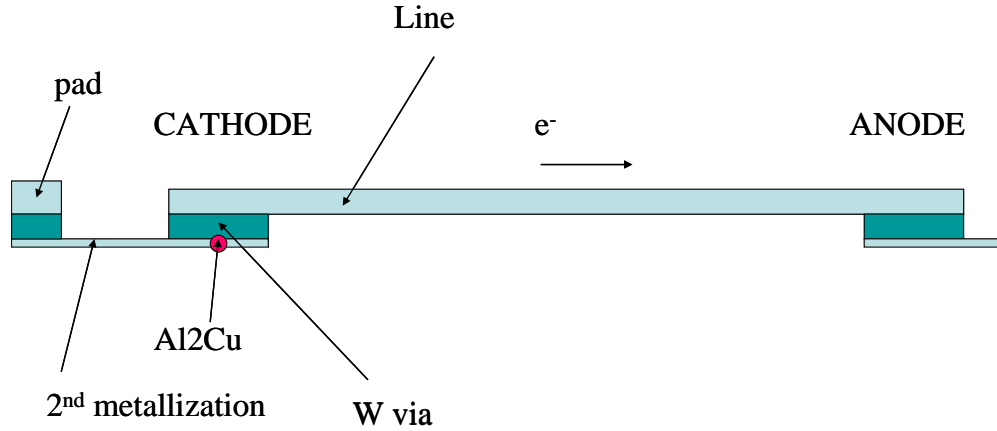


Figure 4. Location of the Al_2Cu precipitate found below the via which connect to the

Precipitates inside the line were too small to be observed by the white beam X-ray microdiffraction technique. However a huge (about 2 micron) Al_2Cu particle was clearly visible in fluorescence and diffraction in the metallization (which has a different aspect ratio than the line) below the via which connect to the pad (Figs. 3, 4). This precipitate appeared after 25 hrs under a current of 30 mA. Although not in the line, this precipitate is still electromigration induced and slowly dissolves after current is turned off. This finding is in agreement with the results of Witt *et al*¹⁸ who also observed precipitates in the contact pad. The proposed mechanism for precipitates growth, dissolution and migration of precipitates is consistent with the results^{3, 4, 18-21} which showed the growth of precipitates at the anode. It explains why the addition of small amounts of Cu to Al conductor lines effectively retards damage of the interconnect line.

Analysis of the orientation of the activated dislocation slip systems shows that the slip systems with dislocation lines almost parallel to the direction of current flow are activated first. Dislocations and dislocation walls cause additional scattering of the electrons by deformation potential related to them. The major part of the interaction potential between electrons and dislocations comes from the deformation field in the matrix around the dislocation, and not from the dislocation core. Around an edge dislocation the deformation field decreases very slowly, as $1/r_{\perp}$ (r_{\perp} is the distance to the dislocation line), leading to a large scattering matrix element. However, scattering only occurs in the direction perpendicular to the dislocation line, because of translation invariance along the dislocation line. The scattering of the electrons can be described as³²

$$(\mathbf{k}_0 - \mathbf{k})\tau = 2\pi m / d_{\tau}, n=0, +(-)1, \dots \quad (12)$$

Here d_{τ} is a lattice parameter along the dislocation line, τ , and k_0, k are impulses of incident and scattered electrons. There exists a strong anisotropy of scattering. The probability of scattering depends on the difference $(k_0 - k)$ as well as on the direction of initial electron momentum k_0 . When almost all unpaired dislocations with the density $n+$ are parallel (as in the case of Al-based interconnects) the anisotropy of scattering becomes essential and electrical properties of the interconnect depend on the direction of the electric current relative to the orientation of dislocation network. Relaxation time of the transverse component of electron's momentum in the presence of a parallel set of edge dislocations with the density $n+$ in the first approximation can be estimated as follows³³

$$\frac{1}{t(k)} = \frac{1}{8} n^+ b^2 \Omega^2 \frac{m}{\hbar^3 k_{\perp}^2} \quad (13)$$

Here t is the time for a single large angle scattering of the electron, Ω is an effective parameter of deformation potential of the edge dislocation, k_{\perp} is a transverse component of electron's momentum, m is the electron mass. The largest scattering occurs in the plane transverse to dislocation line. In the described experiments dislocations are formed in thin Al-based of interconnect under the applied electric field during electromigration. Applied electric field creates additional constraints for dislocations. If a dislocation is formed with the line perpendicular to the applied electric field, scattering of electrons leads to an increased heat dissipation, and such dislocation will be annealed¹⁶. On the other hand, a dislocation network with the lines close to the direction of the electric current creates the smallest resistance for the electric current, and is therefore more likely to persist. When the above slip planes saturates the next possible slip system is activated which has the next smallest inclination angle to the current direction.

CONCLUSIONS

The existence of a coupling between the density of GNDs and the Cu depletion from the cathode is demonstrated. There is practically no plastic activity in the “near anode” end of the line. Our model is consistent with the dissolution, migration and re-growth of Cu rich precipitates, on opposite ends of the interconnect line during electromigration.

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